Molecular production in two-component atomic Fermi gases

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We provide a practical approach to the molecular production via linear downward sweeps of Feshbach resonances in degenerate Fermi gases containing incoherent mixtures of two atomic spin states. We show that the efficiency of the association of atoms is determined just by the Landau-Zener parameter in addition to the density of the gas. Our approach of pairwise summation of the microscopic binary transition probabilities leads to an intuitive explanation for the observed saturation of the molecular production and recovers all atomic loss curves of C.A. Regal *et al.* [Nature (London) **427**, 47 (2003)] as well as K.E. Strecker *et al.* [Phys. Rev. Lett. **91**, 080406 (2003)] without adjustable parameters.

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Ever since the achievement of Bose-Einstein condensation in a dilute vapour of ^{87}Rb atoms, there has been considerable interest in extending the range of species for studies of cold gases. Several experiments [1, 2, 3, 4, 5, 6, 7, 8, 9] have now demonstrated the production of cold molecules via magnetic field tunable Feshbach resonances. One of the techniques relies upon the adiabatic association of pairs of cold atoms to molecules through a linear sweep of a Feshbach resonance level across the zero energy threshold of the colliding atoms. This technique has been applied to atomic Bose-Einstein condensates [4, 5, 9], as well as degenerate two-component Fermi gases [3, 6] containing a balanced incoherent mixture of Zeeman levels of a single atomic species. In contrast to cold Bosons, degenerate Fermions inevitably occupy a range of single particle energy levels up to the Fermi edge. There have been concerns that the spread in collision momenta of Fermionic pairs could prevent an efficient molecular production in an adiabatic sweep. Despite this intrinsic difficulty, a significant molecular conversion of up to approximately 50% of the atoms was reported in Refs. [3, 6], and higher conversion efficiencies have been reported when much slower ramp speeds are used [7, 10]. The few attempts [11, 12, 13, 14] to explain these observations are all based on rather involved field theoretic models. While Refs. [12, 13] provide simulation methods for the molecular production in the presence of Fermi seas, Ref. [11] suggests the maximum molecular production efficiency of 50% in Ref. [3] to be a consequence of a significant temperature dependence of the conversion process.

In this letter we derive a practical universal formula for the molecular production via a linear sweep of the magnetic field strength B in a degenerate two-component Fermi gas in the short time limit where only a single collision of a given atom occurs during the sweep. Our analytic treatment relies upon a pairwise summation of the probabilities for the atomic association, which naturally explains the fast ramp observations of Refs. [3, 6]. We show that the molecular production is largely insensitive to the cold collision momenta and depends only on the product $a_{\rm bg}\Delta B$ of the background scattering length $a_{\rm bg}$ and the resonance width ΔB, in addition to the atomic mass m, the ramp speed $\dot{B}$ as well as the density of the gas. Despite its simplicity, our analytic formula leads to predictions for the molecular production that are virtually indistinguishable from the observations of Refs. [3, 6] within the experimental error bars.

We shall first discuss the association of atomic pairs in the absence of the surrounding gas. A homogeneous magnetic field B splits the atomic hyper-fine angular momentum states into a set of Zeeman levels (f, m_f), labelled by the projection quantum number m_f of the total atomic spin along the axis of the magnetic field and the f value with which it correlates adiabatically at zero field. Indistinguishable Fermions with equal spins are not subject to s-wave scattering and do therefore not contribute to molecular formation. We shall thus consider pairs of atoms whose internal states correspond to different Zeeman levels at asymptotically large inter-atomic separations. We denote the s-wave binary scattering channel of such a pair of unlike Fermions as the entrance channel.

The physical concept of associating a pair of cold atoms is closely related to the variation of its energy spectrum under adiabatic changes of B. Figure 1 shows a coupled channels calculation of these energies for the example of the interacting pairs of ^{40}K atoms in the $(f = 9/2, m_f = -9/2)$ and $(f = 9/2, m_f = -5/2)$ Zeeman states of Ref. [3]. The figure shows that when B varies from high to low fields across the zero energy resonance at $B_0 = 224$ G (1 G$= 10^{-4}$ T), a molecular bound state $\phi_{\rm b}(B)$ appears whose energy $E_{\rm b}(B)$ is indicated by the solid curve. The zero of the binding energy $E_{\rm b}(B)$ coincides with the magnetic field strength B_0 at which the scattering length has a singularity.

The strong magnetic field dependence of the cold interatomic collisions is due to the near degeneracy of the energy $E_{\rm res}(B)$ (dotted dashed line in Fig. 1) of a single closed channel vibrational state $\phi_{\rm res}$ (the Feshbach resonance level) with the threshold for dissociation in the entrance channel (dotted line

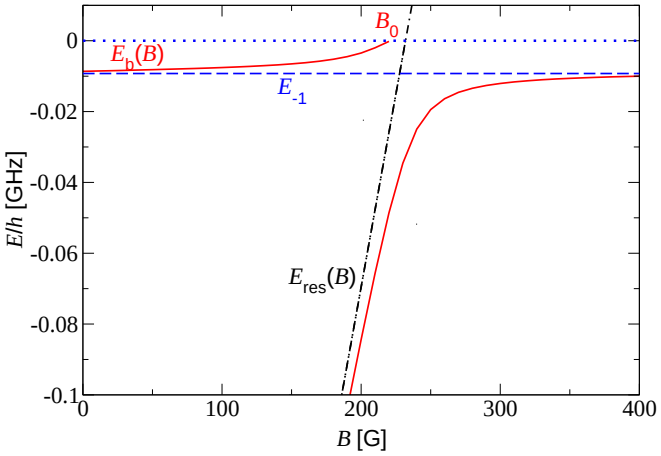

FIG. 1: The binding energy $E_b(B)$ (solid curve) of the highest excited dressed vibrational bound state of a pair of ^{40}K atoms versus the magnetic field strength B in the vicinity of the 224 G zero energy resonance [3]. The zero of energy (dotted line) is chosen, for each magnetic field strength, as the Zeeman energy of a pair of distinguishable Fermions at asymptotically large spatial separation. The zero of the dressed state energy E_b coincides with the singularity of the scattering length in the entrance channel at the magnetic field strength B_0. The dotted dashed line indicates the energy $E_{res}(B)$ of the bare Feshbach resonance state. The dashed line corresponds to the energy E_{-1} of the highest excited bare vibrational level of the entrance channel potential.

in Fig. 1). This allows us to use a two-channel configuration interaction representation [15, 16] in terms of the bare basis states, i.e. the states in the absence of inter-channel coupling. These bare states include the Feshbach resonance level ϕ_{res} and the entrance channel continuum states $\phi_{\mathbf{p}}^{(+)}$ associated with the collision momentum $\mathbf{p}$. The kinetic energy p^2/m as well as the magnetic moment $\mu_{res} = dE_{res}/dB$ of the resonance level are independent of B. Consequently, the determination of the probability for the association of an atom pair with the relative momentum $\mathbf{p}$ can be described by the Landau-Zener approach [15, 16]. We note, however, that although we have chosen a bare state representation, the bound molecules produced in a linear sweep of the magnetic field strength are described by the dressed state $\phi_b(B)$, which accounts for the inter-channel coupling.

The relative momenta in a zero temperature two-component Fermi gas are limited by the maximum of the Fermi momenta of each component, whose associated energy scales are typically on the order of μK (in units of the Boltzmann constant). These energies are too small to be resolved in Fig. 1. In the limited range of cold collision momenta the probability P for the association of a single pair of Fermions in a large sample volume $\mathcal{V}$ is isotropic, i.e. it depends just on the wave number $k = p/\hbar$ associated with the collision momentum $\mathbf{p}$. Neglecting phenomena related to the presence of the surrounding gas, considerations described in Ref. [16] lead to the formula [17]:

$$P(k) = -\frac{(2\pi)^3}{\mathcal{V}}\frac{1}{4\pi k^2}\frac{\partial}{\partial k}\exp\left(-\frac{\mathcal{V}\delta_{LZ}}{3\pi}k^3\right). \quad (1)$$

The inter-atomic interactions enter the probability in terms of the Landau-Zener parameter [15, 16]:

$$\delta_{LZ} = \frac{(2\pi\hbar)^3\left|\langle\phi_{res}|W|\phi_{\mathbf{p}}^{(+)}\rangle\right|^2}{\mathcal{V}|\dot{B}\mu_{res}|} = \frac{4\pi\hbar|a_{bg}\Delta B|}{\mathcal{V}m|\dot{B}|}. \quad (2)$$

Here $W(r)$ is the potential describing the inter-channel coupling. We note that $\langle\phi_{res}|W|\phi_{\mathbf{p}}^{(+)}\rangle$ and consequently δ_{LZ} are independent of k provided that $|a_{bg}|$ is sufficiently small to satisfy the relation $k|a_{bg}| \ll 1$. The k dependence of Eq. (1) is due to downward transitions into lower energetic continuum states that compete with the molecular formation in an isolated two-body system [15].

We shall show in the following that the molecular production in the limit of fast magnetic field ramps as well as in the opposite saturation limit can be determined in a straightforward manner, provided that multiple collisions of a given atom can be neglected. To this end, we shall first consider the limit of ramp speeds sufficiently high that Eq. (1) is well approximated by first order perturbation theory in the inter-channel coupling. A linear expansion of Eq. (1) in δ_{LZ} then shows that $P(k)$ is independent of k, and reduces to the linearised Landau-Zener formula for a single curve crossing [15, 16]:

$$P = 2\pi\delta_{LZ}. \quad (3)$$

Despite the fact that the association of a given atom pair in the large sample volume $\mathcal{V}$ is a rare event, the molecular production in an incoherent mixture of N Fermions can be rather efficient because each of the N_1 atoms in one of the spin states has all N_2 atoms of the other component to interact with. In accordance with classical probability theory, the total number N_b of diatomic molecules in the state ϕ_b is given by the pairwise incoherent sum of the microscopic transition probabilities:

$$N_b = N_1 N_2 P. \quad (4)$$

Here N_1N_2 is the number of pairs of unlike atoms. Equations (3) and (4) then lead to the following fraction of atoms associated to molecules:

$$2N_b/N = 2\alpha(1-\alpha)NP = 2\alpha(1-\alpha)\left[2\pi n\mathcal{V}\delta_{LZ}\right]. \quad (5)$$

Here $n = N/\mathcal{V}$ is the local density and α is the minimum of the fractions N_1/N and N_2/N. Since $\mathcal{V}\delta_{LZ}$ is independent of $\mathcal{V}$, Eq. (5) depends just on the local density of the gas. The pre-factor $\alpha(1-\alpha)$ accounts for the size of the sub-ensemble of pairs of unlike Fermions and the factor of two indicates the number of atoms per molecule, while $2\pi n\mathcal{V}\delta_{LZ}$ can be interpreted as a density dependent Landau-Zener transition probability [15, 16].

The pairwise summation of microscopic transition probabilities is justified when the number of molecules produced

is small in comparison to the total number of atoms [16, 18]. In this limit of high ramp speeds the molecular production does not crucially depend on the presence of the Fermi seas. As the ramp speed decreases, Eq. (1) becomes momentum dependent, since, unlike for fast ramps, there can be decay during the ramp to lower energy continuum states of the two-body system with $E > 0$. In the presence of the surrounding two-component Fermi gas, however, these downward transitions would lead into occupied modes and are therefore prevented. In order to extend Eq. (5) to lower ramp speeds, we shall thus follow the approach of Refs. [15, 16] and replace the density dependent linearised Landau-Zener formula $2\pi n\mathcal{V}\delta_{\rm LZ}$ by the complete Landau-Zener transition probability $1-\exp(-2\pi n\mathcal{V}\delta_{\rm LZ})$ for a linear curve crossing in the absence of downward transitions to other continuum states. The corrections to this procedure involve the dynamic depletion of the available pairs during the atomic association. Comparisons between genuinely many-body approaches and the Landau-Zener formula [16] for the case of a condensate of identical Bosons show that the dynamic depletion of the pairs changes the functional dependence of the molecular production efficiency on the ramp speed. The absolute magnitude of these corrections, however, is typically small in comparison with the total depletion of the atoms and can be neglected. The molecular production efficiency in a two-component Fermi gas may thus be approximated by:

$$\frac{2N_{\rm b}}{N} = 2\alpha(1-\alpha)\left[1-\exp\left(-n\frac{8\pi^2\hbar|a_{\rm bg}\Delta B|}{m|\dot{B}|}\right)\right]. \qquad (6)$$

The molecular production efficiency can not exceed 50%, given the ansatz in Eq. (6). This limit is quite intuitive as, given only one chance to associate, a Fermion in the larger one of the two components can find an interacting partner with a probability of 1/2 at best. The saturated efficiency in mixtures with unbalanced populations of the spin components can only be lower and is given by $2\alpha(1-\alpha)$. The exponential function in Eq. (6) provides a smooth interpolation between the straightforward asymptotic limits of the ramp speed.

The range of validity of our approach is set by the assumption that only a single collision of a given atom can occur during the association process. When the ramp speed is chosen sufficiently low for multiple collisions to become significant, efficiencies exceeding 50% can result [7, 10] from the same physical mechanisms that can convert an atomic gas to a molecular gas at constant magnetic field strength [8, 19, 20]. To this end, the experiments of Ref. [10] applied magnetic field ramps at least ten times slower than the slowest ramp of Ref. [3] for Feshbach resonance parameters and densities comparable to those of Ref. [3].

To compare the predictions of Eq. (6) to the experimental results of Refs. [3, 6], we have applied the local density approximation, i.e. we have averaged Eq. (6) in accordance with the density distribution of the trapped gases. We have determined the density profiles from the zero temperature Thomas-Fermi approximation [21], adapted to the experimental trap geometries. Figure 2 shows the number $N-2N_{\rm b}$ of free ^{40}K

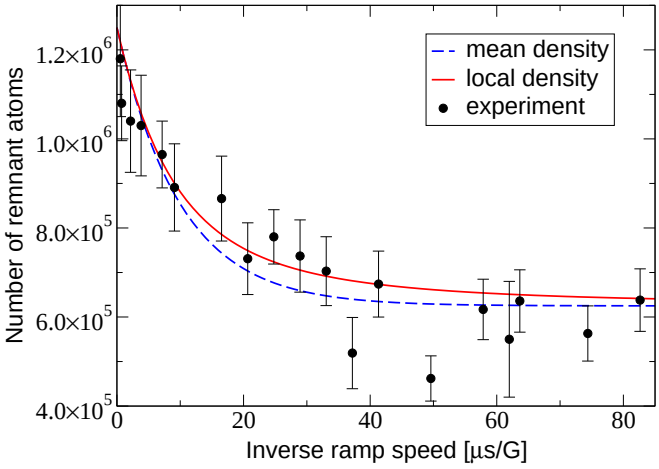

FIG. 2: The number of atoms remaining versus the inverse ramp speed $1/\dot{B}$ for a linear sweep of the magnetic field strength across the 224 G zero energy resonance in a two-component Fermi gas of ^{40}K. The experimental data of Ref. [3] (circles) are compared to the results of the pairwise summation approach of Eq. (6) with $\alpha = 1/2$. The solid and dashed curves indicate local and mean density approximations, respectively.

atoms remaining in the experiments of Ref. [3] as compared to the predictions of Eq. (6). We have estimated the total number of atoms to be $N = 1.25\times10^6$ (cf. Fig. 2) and used the background scattering length $a_{\rm bg} = 174\,a_0$ [22] ($a_0 = 0.052918$ nm), the resonance width $\Delta B = 9.7$ G [22], and the radial angular trap frequency $\omega_{\rm r} = 2\pi\times215$ s^{-1}, which, together with the aspect ratio of 70 [3], largely recover the experimental peak density of $n_{\rm pk} = 1.4\times10^{13}$ cm^{-3} [3]. This procedure yields a mean density of $n = 9\times10^{12}$ cm^{-3}. The predictions of the mean and local density approaches to Eq. (6) clearly follow the slope as well as the magnitude of the experimental data. We obtain a similar agreement with unpublished lower density ($n_{\rm pk} = 9\times10^{12}$ cm^{-3}) data of Regal *et al.* [23].

To further confirm the validity of Eq. (6), Fig. 3 shows an analogous comparison with the results of Ref. [6]. In these experiments the molecules were produced by a linear sweep of the magnetic field strength across the 543 G zero energy resonance of ^{6}Li in the entrance channel associated with the set of quantum numbers ($f = 1/2, m_f = +1/2$) and ($f = 1/2, m_f = -1/2$) of the interacting atoms. We have performed an exact coupled channels calculation to determine the resonance parameters. From these considerations we obtain $|a_{\rm bg}\Delta B| = 5.916\,a_0$G. The Thomas-Fermi density profile used in the local density approach is determined by the Fermi energy $E_{\rm F}$, which in the case of the combined harmonic and box-like trapping potential of Ref. [6] is given by $E_{\rm F} = \left[15\pi N\hbar^3\omega_{\rm r}^2/(8\sqrt{2m}L)\right]^{2/5}$. Here $\omega_{\rm r} = 2\pi\times800$ s^{-1} is the angular frequency of the radial harmonic trap and $L = 480\,\mu$m is the size of the axial box-like potential [6]. This leads to a mean density of $n = 4\times10^{12}$ cm^{-3}.

The agreement with the experimental data in Figs. 2 and

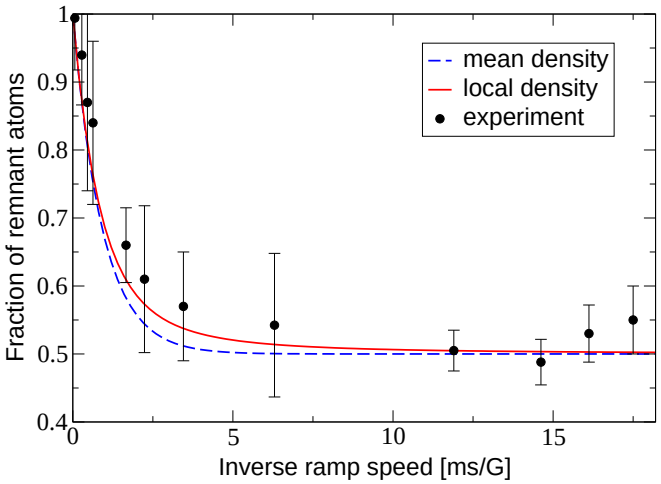

FIG. 3: The fraction $1 - 2N_b/N$ of remnant atoms versus the inverse ramp speed $1/\dot{B}$ for a linear sweep of the magnetic field strength across the 543 G zero energy resonance in a two-component Fermi gas of ^{6}Li. The circles indicate the experimental data of Ref. [6]. The solid and dashed curves are predictions of Eq. (6) with $\alpha = 1/2$ in the local and mean density approximations, respectively.

3 suggests that the pairwise summation approach recovers all the relevant aspects of the physics involved. This implies that the molecular production efficiency is determined by the density of the gas, the ramp speed and the atomic mass, in addition to a single universal parameter of the resonance enhanced collision physics, the product of the background scattering length and the resonance width. The density profile provides a direct dependence of the molecular production on the Fermi statistics. Our results indicate, however, that even a mean density approximation yields a rather useful estimate of the number of molecules produced. Our ansatz provides an excellent approximation for the molecular production efficiency in the limit of very fast downward sweeps of the Feshbach resonance level in two-component Fermi gases and gives a 50% efficiency as a natural limit, provided that phenomena related to multiple collisions of a given atom are negligible. The pairwise summation approach has a rather wide range of applicability in dilute gases, including cold Bosons [15, 16, 18] and Fermions as well as their mixtures. The main requirement is the diluteness of the gas in combination with a binary transition, which is sufficiently fast that multiple collisions can be neglected. Such a binary transition may be realised by a single linear sweep of the magnetic field strength, but it can as well involve fast sequences of magnetic field pulses [18] applied in the experiments of Refs. [1, 2].

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